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Landé *g* factors for $2p^4$ (^{3}P)3p and $2p^4$(^{3}P)3d states of Ne II☆

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Abstract

The Landé *g* factor characterizes the Zeeman effect, caused by the interaction of the magnetic moment of an atom and an external magnetic field. This factor is largely unaffected by correlation but depends strongly on the mixing of terms. In this paper the Landé *g* factors for the $2p^4$(^{3}P)3p and $2p^4$(^{3}P)3d terms of Ne II are reported, computed from multiconfiguration Dirac–Fock and multiconfiguration Hartree–Fock plus Breit–Pauli wave functions. Extensive term mixing is present for some of the terms of $2p^4$(^{3}P)3d. It is shown how the g_J factor, which provides coupling information, can be used to identify MCDF wave functions.

Keywords: Landé *g* factor; Zeeman effect; Multiconfiguration Dirac–Fock; Multiconfiguration Hartree–Fock + Breit–Pauli

1. Introduction

The *Handbook of Atomic Data*, published by Fraga et al. [1], reports many atomic properties based on a Dirac–Fock–Breit–Pauli–Hartree–Fock method. Included in the book are Landé *g* factors of a few levels, but not many. The *g* factors are associated with the Zeeman effect and determine energy splittings in an external magnetic field. Unlike many other atomic properties, they are not as affected by correlation as by term mixing. In this paper, we explore the determination of Landé *g* factors in both the intermediate coupling multiconfiguration Hartree–Fock Breit–Pauli approximation and the multiconfiguration Dirac–Fock–Breit approximation. For convenience we will refer to these simply as MCHF and MCDF, respectively. Our investigation is restricted to the $2p^4$(^{3}P)3p and $2p^4$(^{3}P)3d states of Ne II, a system investigated recently in both methodologies for the purpose of the study of transition rates. Extensive term-mixing was found, particularly for the $2p^4$(^{3}P)3d even states [2]. It is suggested that the *g* factor may be used in labeling of states computed in the multiconfiguration Dirac–Fock–Breit formalism.

2. Theory

In the non-relativistic MCHF approach [3,4], the wave function ψ for a state labeled γLS, where γ represents the configuration and any other quantum numbers required to specify the state, is expanded in terms of configuration state functions (CSFs) with the same *LS* term,

$$\psi(\gamma LS) = \sum_j c_j \Phi(\gamma_j LS). \quad (1)$$

The configuration state functions $\Phi(\gamma LS)$ are antisymmetrized linear combinations of products of

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spin-orbitals

$$\phi_{nlm_lm_s} = \frac{1}{r} P_{nl}(r) Y_{lm_l}(\theta, \varphi) \xi_{m_s}(\sigma), \tag{2}$$

where the radial functions $P_{nl}(r)$ are represented by their numerical values on a logarithmic grid, $Y_{lm_l}(\theta, \varphi)$ is a spherical harmonic, and $\xi_{m_s}(\sigma)$ a spin-function. The radial functions are required to be orthonormal within each l symmetry. The multiconfiguration self-consistent field (MC-SCF) procedure is used to optimize both the orbitals and the expansion coefficients to self-consistency.

Once a set of radial functions has been obtained, a Breit–Pauli configuration interaction (CI) calculation can be performed where the wave function is expanded in *LSJ* coupled configuration state functions

$$\psi(\gamma LSJ) = \sum_j c_j \Phi(\gamma_j L_j S_j J). \tag{3}$$

Now only the expansion coefficients are to be determined. This is done by diagonalizing the Hamiltonian matrix with respect to the Breit–Pauli operator, which includes the most important, lowest-order corrections of the Dirac–Coulomb–Breit operator [4]. All MCHF calculations used the MCHF atomic structure package [3], modified for large-scale computation. This is the intermediate coupling or LSJ approximation.

In the MCDF approach [5], the wave function ψ for a state labeled γJ, where γ represents the configuration and any other quantum numbers required to specify the state, is approximated by an expansion over *jj* coupled configuration state functions

$$\Psi(\gamma J) = \sum_j c_j \Phi(\gamma_j J). \tag{4}$$

The configuration state functions $\Phi(\gamma J)$ are antisymmetrized linear combinations of products of relativistic orbitals

$$\phi_{n\kappa m} = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r) \chi_{\kappa m}(\hat{r}) \\ \mathrm{i} Q_{n\kappa}(r) \chi_{-\kappa m}(\hat{r}) \end{pmatrix}. \tag{5}$$

Here κ is the relativistic angular quantum number, $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small component radial wave functions and $\chi_{\kappa m}(\hat{r})$ is the spinor spherical harmonic in the *lsj* coupling scheme

$$\chi_{\kappa m}(\hat{r}) = \sum_{m_l, m_s} \langle l \tfrac{1}{2} m_l m_s | jm \rangle Y_{lm_l}(\theta, \varphi) \xi_{m_s}(\sigma). \tag{6}$$

As for MCHF the radial functions $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are represented on a logarithmic grid and are required to be orthonormal within each κ symmetry. In the multiconfiguration self-consistent field procedure both the radial functions and the expansion coefficients for the configuration state functions are optimized to self-consistency under additional conditions on the large and small component radial functions at the vicinity of the nucleus to avoid collapse into the negative energy continuum [6].

Once a set of radial orbitals has been obtained, relativistic configuration interaction (RCI) calculations can be performed. Here the transverse photon interaction

$$\mathscr{H}_{\mathrm{trans}} = -\sum_{i<j}^{N} \left[\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j \cos(\omega_{ij} r_{ij})}{r_{ij}} + (\boldsymbol{\alpha}_i \cdot \nabla_i)(\boldsymbol{\alpha}_j \cdot \nabla_j) \frac{\cos(\omega_{ij} r_{ij}) - 1}{\omega_{ij}^2 r_{ij}} \right] \tag{7}$$

may be included in the Hamiltonian. The photon frequency ω_{ij} used by the RCI program in calculating the matrix elements of the transverse photon interaction is taken to be the difference in the diagonal Lagrange multipliers ϵ_i and ϵ_j associated with the orbitals. In general, diagonal Lagrange multipliers are approximate electron removal energies only when orbitals are spectroscopic and singly occupied. Thus it is not known how well the code can determine the full transverse photon interaction when correlation orbitals are present. What can be obtained instead is the low frequency limit $\omega_{ij} \rightarrow 0$ usually referred to as the Breit interaction.

3. Method of computation

In both cases we used systematic, large-scale methods where expansions are obtained from rules for distributions of electrons to orbitals, and orbital sets are allowed to grow in size.

In many respects, the MCDF calculations are conceptually the more straightforward. The results are totally ab initio: relativistic effects are included directly, but because of the *jj* coupling, there are about twice as many orbitals and expansions growing so rapidly that not nearly as much correlation can be included. On the other hand, the MCDF codes [7,8]

have been modified to deal with independent J-blocks and orbitals can be optimized simultaneously on a number of different levels. In all cases, the expansions were over the CSFs from the distribution $1s^2\{2\}^5\{2,3,\ldots,n\}^2$, where n is the maximum principal quantum number of the orbital set, but with $n \leq 5$. The distribution denotes all possible configuration states with a filled $1s^2$ core, followed by five orbitals that are either 2s, 2p+ or 2p−, with the remaining two orbitals restricted to the orbital set as determined by the largest principal quantum number n. The latter parameter characterizes the orbital set. A set of 1s, 2s, 2p+, 2p− orbitals, both for the odd and the even parity states, was obtained from an extended optimal level MCDF calculation for $2s^22p^4\,^3P_{0,1,2}$, optimizing simultaneously on all three levels. Then, as new orbitals were included successively for $n = 3$, $n = 4$, and $n = 5$ orbital sets, only the new orbitals were varied. Details of the optimization procedure and the resulting spectrum can be found in Ref. [2].

The MCHF method with Breit–Pauli corrections is quite different. In fact it is not unlike a basis set method where the variational calculations determine a set of orbitals that must simultaneously describe the levels of particular interest. In the case of $2p^4(^3P)3p$ the possible terms are ^4D, ^4P, ^4S, ^2D, ^2P, and ^2S. In the present work, the lower lying $2p^5\ ^2P$ is not of interest and need not be optimized. In this work, the optimization process was somewhat arbitrary and did not use the simultaneous optimization scheme developed later, specifically for such cases where an orbital basis is optimized simultaneously on selected terms and even selected eigenvalues [9]. The final expansion for each term was then generated as the union of the two distributions, $1s^2\{2\}^4\{2,3\}\{2,3,4\}^2$ and $1s^2\{2\}^5\{2,3,4,5,6\}^2$. Note that more correlation is included with this approach, not only because the largest orbital sets included those with $n = 6$, but also because the first distribution included more excitations.

For $2p^4(^3P)3d$ the set of possible terms of interest are ^4F, ^4D, ^4P, ^2F, ^2D, and ^2P. In addition to the lower-lying $2s2p^6\ ^2S$ term, there are all the $2p^43s$ terms which will interact with the levels of interest. Though they need not be carefully optimized, they should be well enough represented in the basis to reproduce the spectrum. Again, the details of optimization can be found elsewhere [2]. Expansions were obtained for each term of interest along with ^2G and ^2S, which have J-values in common with these terms. These were then combined in Breit–Pauli calculations for the different J-values.

In a Breit–Pauli calculation, the accuracy of a wave function can be enhanced considerably by shifting the diagonal LS energies for each block. In the odd parity case, the critical J-value was the $J = 3/2$. To bring these $J = 3/2$ levels into agreement with observation, as tabulated by Persson [10], the diagonal LS energies were adjusted. These shifts were determined after a Breit–Pauli calculation was performed without any adjustments and then compared with observation. Not only did the shifts improve the separation between levels, they also brought the levels into position relative to the energy of the ground state. For the even-parity case, at first it seemed appropriate to adjust the diagonals for the most critical $J = 3/2$ levels, or $J = 5/2$ for ^2F. However, such an adjustment process assumes the labels assigned by Persson [10] are correct. Instead, it was decided to shift the blocks by choosing J values for which mixing would not be strong, thereby determining the appropriate labeling. The results suggested that the levels designated by Persson as $^4F_{7/2}$ and $^2F_{7/2}$ should be reversed [2].

Once the wave functions have been determined, various properties can be determined, including the Landé g factor that is connected with the Zeeman effect.

4. Zeeman effect

The Zeeman effect is caused by the interaction between the magnetic moment of the atom and an external magnetic field. The operator representing this interaction is

$$\mathscr{H}_m = -\boldsymbol{\mu}\cdot\mathbf{B}, \tag{8}$$

where $\boldsymbol{\mu}$ is the magnetic moment and $\mathbf{B}$ the magnetic field. In the Breit–Pauli approximation there are two contributions to the magnetic moment; one from the orbital motions and the other from the spin motions of the electrons. Adding these two contributions we have

$$\boldsymbol{\mu} = -\mu_B(\mathbf{L} + g_s\mathbf{S}), \tag{9}$$

where μ_B is the Bohr magneton and $g_s = 2.00232$, the

g factor of the spin corrected for quantum electrodynamic (QED) effects.

If the external field is weak such that the magnetic interaction energy is small compared to the fine-structure separations, $\mathscr{H}_m$ can be treated in first-order perturbation theory with wave functions from the Breit–Pauli Hamiltonian as zero-order functions. Choosing the direction of the external field as the z-direction, the operator for the interaction can be written

$$\mathscr{H}_m = \mu_B B(L_z + g_s S_z), \tag{10}$$

and the energy level γJ is split according to

$$\Delta E(\gamma JM_J) = \langle \gamma JM_J|\mathscr{H}_m|\gamma JM_J\rangle = \mu_B B\langle \gamma JM_J|L_z + g_s S_z|\gamma JM_J\rangle. \tag{11}$$

In the multiconfiguration Breit–Pauli approximation this becomes

$$\Delta E(\gamma JM_J) = \mu_B B \sum_{j,k} c_j c_k \langle \Phi(\gamma_j L_j S_j JM_J)|L_z + g_s S_z|\Phi(\gamma_k L_k S_k JM_J)\rangle. \tag{12}$$

The matrix elements between the CSFs are readily evaluated to yield

$$\langle \Phi(\gamma LSJM_J)|L_z + g_s S_z|\Phi(\gamma' L'S'JM_J)\rangle = \delta_{\gamma\gamma'}\delta_{LL'}\delta_{SS'}g_J(LS)M_J, \tag{13}$$

where

$$g_J(LS) = 1 + (g_s - 1)\frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \tag{14}$$

is the Landé g factor without any term mixing, i.e. in pure LS coupling. Summing up, the energy splitting can now be written

$$\Delta E(\gamma JM_J) = g_J(LSJ)\mu_B BM_J, \tag{15}$$

where

$$g_J(LSJ) = \sum_j c_j^2 g_J(L_j S_j) \tag{16}$$

is the Landé g factor in intermediate coupling. In theoretical studies this quantity can be used as a valuable probe of the coupling conditions in the atom.

Since the energy splitting is proportional to M_J the operator $\mathscr{H}_M$ can be replaced with

$$\mathscr{H}_M = g_J(LSJ)\mu_B \mathbf{J}\cdot\mathbf{B}. \tag{17}$$

This equivalent operator establishes the connection with the fully relativistic case. In the relativistic theory the interaction with the magnetic field is given by

$$\mathscr{H}_m = \sum_{j=1}^{N} \boldsymbol{\alpha}_j\cdot\left(\tfrac{1}{2}\mathbf{B}\times\mathbf{r}_j\right). \tag{18}$$

The interaction can also be written as a scalar product

$$\mathscr{H}_m = \tfrac{1}{2}\mathbf{N}\cdot\mathbf{B}, \tag{19}$$

where

$$N_q^{(1)} = -\sum_{j=1}^{N} \mathrm{i}\sqrt{\frac{8\pi}{3}}\, r_j \boldsymbol{\alpha}_j\cdot Y_{1q}^{(0)}(\hat{r}_j) \tag{20}$$

is an operator of the same tensorial form as the magnetic dipole hyperfine operator [11]. Expressing the operator $\mathscr{H}_M$ in the equivalent form

$$\mathscr{H}_m = g_J(jj)\mu_B \mathbf{J}\cdot\mathbf{B} \tag{21}$$

and using the projection theorem gives the Landé g factor in jj coupling

$$g_J(jj) = \frac{1}{2\mu_B}\frac{\langle \gamma_J J\|N^{(1)}\|\gamma_J J\rangle}{\sqrt{J(J+1)(2J+1)}}. \tag{22}$$

In the relativistic Dirac theory the electron g factor is exactly 2. The QED corrections to this factor leads to a correction of the interaction operator

$$\Delta\mathscr{H}_m = \frac{(g_s - 2)}{2}\mu_B \beta\boldsymbol{\Sigma}\cdot\mathbf{B}, \tag{23}$$

where $\boldsymbol{\Sigma}$ is the relativistic spin matrix. Defining the operator $\Delta\mathbf{N}$ by

$$\Delta N_q^{(1)} = \sum_{j=1}^{N} \beta_j \boldsymbol{\Sigma}_{qj} \tag{24}$$

then the correction to the Landé g factor is given by (see Ref. [11] for details)

$$\Delta g_J(jj) = \frac{(g_s - 2)}{2}\frac{\langle \gamma_J J\|\Delta\mathbf{N}^{(1)}\|\gamma_J J\rangle}{\sqrt{J(J+1)(2J+1)}}. \tag{25}$$

The evaluation of the matrix elements in jj coupling was done by a modified version of the hyperfine

Table 1
Comparison of Landé g factors for $2p^4(^3P)3p$ states of Ne II

Level	$g_J(LS)$	$g_J(LSJ)$	$g_J(jj)$
$^4D^0_{7/2}$	1.42956542	1.42956541	1.42829857
$^4P^0_{5/2}$	1.60139158	1.59983083	1.59806312
$^4D^0_{5/2}$	1.37229003	1.36994419	1.36863839
$^2D^0_{5/2}$	1.20046386	1.20431663	1.20393627
$^4P^0_{3/2}$	1.73503416	1.73317402	1.73106887
$^4D^0_{3/2}$	1.20046386	1.19934977	1.19875118
$^2D^0_{3/2}$	0.79953614	0.80635674	0.80569633
$^4S^0_{3/2}$	2.00231930	2.00009455	1.99814034
$^2P^0_{3/2}$	1.33410643	1.33225344	1.33175896
$^4P^0_{1/2}$	2.67053217	2.66564528	2.66115147
$^4D^0_{1/2}$	−0.00231930	0.00163534	0.00426238
$^2S^0_{1/2}$	2.00231930	1.93165792	1.96752766
$^2P^0_{1/2}$	0.66589357	0.73737916	0.69935731

structure program [12] belonging to the MCDF program package.

5. Results

Tables 1 and 2 show the g factor computed in different ways: $g_J(LS)$ is the single term value, $g_J(LSJ)$ is the intermediate coupling value, and $g_J(jj)$ is the QED corrected value as determined from a multiconfiguration Dirac–Fock–Breit calculation.

Table 2
Comparison of Landé g factors for $2p^4(^3P)3d$ states of Ne II

Level	$g_J(LS)$	$g_J(LSJ)$	$g_J(jj)$
$^4F_{9/2}$	1.33410643	1.33405411	1.33312145
$^4D_{7/2}$	1.42956542	1.42130719	1.41954265
$^4F_{7/2}$	1.14318847	1.17752104	1.17693132
$^2F_{7/2}$	1.23864745	1.21246467	1.21249501
$^4D_{5/2}$	1.37229003	1.36852514	1.36735537
$^2D_{5/2}$	1.20046386	1.13139412	1.13159673
$^4F_{5/2}$	1.02863769	1.06474261	1.06987276
$^2F_{5/2}$	0.85681153	0.95599475	1.08781012
$^4P_{5/2}$	1.60139158	1.53883417	1.40175128
$^4D_{3/2}$	1.20046386	1.20352656	1.20344693
$^2D_{3/2}$	0.79953614	0.85208847	0.86740242
$^4F_{3/2}$	0.39860842	0.74977631	1.39391237
$^4P_{3/2}$	1.73503416	1.36136564	0.707083489
$^2P_{3/2}$	1.33410643	1.30088570	1.296989299
$^4D_{1/2}$	−0.00231930	0.03875369	0.045329737
$^4P_{1/2}$	2.67053217	2.59146263	2.591722837
$^2P_{1/2}$	0.66589357	0.70380560	0.697122022

In order to interpret these results we present, in Table 3, the term mixing of the states of interest, in the Breit–Pauli approximation.

For the $2p^4(^3P)3p$ states the mixing of terms is relatively small, the largest occurring for $^2P^0_{1/2}$. This is also the state where term mixing has produced the largest change in the g_J factor. It also needs to be pointed out that whereas $g_{1/2}(^4D)$ is negative, the small admixture of other $J = 1/2$ states has produced a positive Landé factor.

The situation for $2p^4(^3P)3d$ states is somewhat different. On the whole, there is excellent agreement between the intermediate coupling and MCDF g_J values, even when term mixing has resulted in a significant difference with $g_J(LS)$. But some discrepancies are observed. An example can be found in $^2F_{5/2}$ and $^4P_{5/2}$. These terms are relatively close to each other, being separated by only 145.44 cm^{-1} in the observed spectrum. The MCDF separation was 138.44 cm^{-1}, whereas the MCHF Breit–Pauli separation was 252.63 cm^{-1}. In this case, we expected MCDF transition rates from these levels to be the more accurate, yet the agreement in the g_J values is good. But there is another interesting situation: $^4F_{3/2}$ and $^4P_{3/2}$. In this case, the separation is 42.43, 53.91, and 51.58 cm^{-1}, respectively, for observed, MCDF, and intermediate coupling Breit–Pauli. In classifying the energy levels of the $J = 3/2$ states, the MCDF states were assigned a label by order of their computed energy, consistent with observed and with Breit–Pauli values. A comparison of the g_J values shows that the two states are interchanged if ordered according to their g_J values.

Relabeling the MCDF wave function according to the g_J value removes an anomaly found in the transition data [2]. Table 4 compares the MCDF and MCHF + Breit–Pauli results, with the label of the former interchanged. By no means is the agreement excellent but now the two calculations have the same dominant decay mechanism. Values of F_{ul} give the rate of decay of a transition rate relative to the largest transition rate. For both methodologies the dominant decay is $^4P_{3/2} - {}^4S^0_{3/2}$ and $^4F_{3/2} - {}^4D^0_{1/2}$ for the two upper states, respectively.

Griesman et al. [13] have reported branching fractions and transition probabilities for some of these levels. In our earlier publication [2], some branching ratios for decay from $^4P_{3/2}$, using the energy ordered

Table 3
Major Breit–Pauli contributions to the wave function expansion. Persson's term designation in used. Unless indicated otherwise, the $2p^4$ term of the target is always ^3P

State	Contribution to the expansion				
$2p^4(^3P)3p$					
$^4P^0_{5/2}$	0.984 $^4P^0$				
$^4P^0_{3/2}$	0.983 $^4P^0$				
$^4P^0_{1/2}$	0.986 $^4P^0$				
$^4D^0_{7/2}$	0.988 $^4D^0$				
$^4D^0_{5/2}$	0.976 $^4D^0$	−.142 $^2D^0$			
$^4D^0_{3/2}$	0.982 $^4D^0$				
$^4D^0_{1/2}$	0.987 $^4D^0$				
$^2D^0_{5/2}$	0.977 $^2D^0$	0.140 $^4D^0$			
$^2D^0_{3/2}$	0.980 $^2D^0$				
$^2S^0_{1/2}$	0.960 $^2S^0$	0.211 $^2P^0$			
$^4S^0_{3/2}$	0.984 $^4S^0$				
$^2P^0_{3/2}$	0.923 $^2P^0$	−0.300 (^{1}D)$^2P^0$			
$^2P^0_{1/2}$	0.898 $^4P^0$	−0.300 (^{1}D)$^2P^0$	−0.288 ^2S		
$2p^4(^3P)3d$					
$^4D_{7/2}$	0.968 ^4D	0.173 ^4F			
$^4D_{5/2}$	0.962 ^4D	0.157 ^4F	0.151 ^4P		
$^4D_{3/2}$	0.964 ^4D	0.161 ^4P	0.109 ^4F		
$^4D_{1/2}$	0.975 ^4D	−0.115 ^2P	0.108 ^4P		
$^4F_{9/2}$	0.989 ^4F				
$^4F_{7/2}$	0.792 ^2F	−0.591 ^4F			
$^2D_{5/2}$	0.815 ^2D	0.426 ^2F	−0.320 ^4F	0.169 ^4P	
$^2D_{3/2}$	0.868 ^2D	−0.311 ^4F	0.249 ^2P	0.242 ^4P	
$^2F_{7/2}$	0.774 ^4F	0.585 ^2F	−0.192 ^4D		
$^4P_{1/2}$	.970 ^4P	.168 ^2P			
$^4F_{5/2}$	0.850 ^4F	0.432 ^2D	−0.209 ^2F	−0.130 ^4D	
$^4F_{3/2}$	0.832 ^4F	0.470 ^4P	0.156 ^2P	−0.151 ^4D	0.135 ^2D
$^4P_{3/2}$	0.810 ^4P	−0.418 ^4F	−0.365 ^2D	−0.114 ^4D	
$^2F_{5/2}$	0.847 ^2F	0.356 ^4F	−0.269 ^4P	−0.243 ^2D	
$^4P_{5/2}$	0.919 ^4P	−0.258 ^2D	0.189 ^2F	−0.167 ^4D	
$^2P_{1/2}$	0.967 ^2P	−0.156 ^4P	0.131 ^4D		
$^2P_{3/2}$	0.942 ^2P	−0.259 ^2D	−0.126 ^4P		

MCDF labels, were incorrectly compared with values for $^4F_{3/2}$. Table 5 reports the branching ratios for this term, using the label from the g_J values for both MCDF and MCHF + Breit–Pauli. Since the latter is based on shifted energy values, the levels are in good agreement with those observed. In the NIST column, there is substantial disagreement with both MCDF and MCHF for the decay to $^4S^0_{3/2}$, a transition arising from term mixing. Unlike some transitions which are spin-forbidden, this one is "L" (or angular) forbidden and, intuitively, one would expect it not to be as large as observed by Griesman et al. [13]. In the MCDF column, there is a large branching factor to $^4D^0_{3/2}$, neither reproduced by MCHF calculations nor observed in the experiment. As mentioned earlier, the MCDF calculations did not include as much correlation. In particular, correlation within $2p^4$ was neglected. When levels of the same J are so closely spaced, more correlation may be needed. In some respects, the agreement between MCHF and observation is better.

6. Conclusions

The Landé g factor is not as sensitive to correlation within a term as to the mixing of terms. Thus it seems to be a means of identifying an MCDF wave function,

Table 4
MCDF and MCHF transition energies (in cm^{-1}), transition rates (in s^{-1}), and relative branching factors. In the case of MCDF data, results in the Coulomb (velocity) gauge are given above those of the Babushkin (length) gauge. Persson's labels are used

Upper level	Lower level	ΔE	MCDF			ΔE	MCHF		
			A_{ul}	gf	F_{ul}		A_{ul}	gf	F_{ul}
$^4P_{3/2}$	$^4S^0_{3/2}$	28288.0	1.367D+08	1.0244	100.00	28045.0	1.004D+08	0.7656	100.00
			1.304D+08	0.9770	100.00				
	$^4P^0_{5/2}$	34831.4	2.781D+07	0.1374	20.34	34803.9	4.654D+07	0.2304	46.35
			2.999D+07	0.1482	23.00				
	$^4P^0_{3/2}$	34612.4	1.633D+06	0.0082	1.19	34584.1	7.009D+06	0.0351	6.98
			1.417D+06	0.0071	1.09				
	$^4P^0_{1/2}$	34432.3	5.342D+07	0.2702	39.08	34403.6	6.957D+07	0.3525	69.28
			5.858D+07	0.2963	44.93				
	$^4D^0_{5/2}$	31740.8	1.641D+07	0.0977	12.00	31545.8	2.296D+05	0.0014	0.23
			2.042D+07	0.1215	15.66				
	$^4D^0_{3/2}$	31495.1	2.650D+05	0.0016	0.19	31302.2	4.177D+07	0.2557	41.60
			9.013D+04	0.0005	0.07				
	$^4D^0_{1/2}$	31353.5	9.818D+07	0.5989	71.82	31160.4	2.475D+07	0.1528	24.65
			1.058D+08	0.6452	81.12				
	$^2S^0_{1/2}$	28427.8	8.198D+05	0.0061	0.60	28218.1	1.851D+06	0.0139	1.84
			8.004D+05	0.0059	0.61				
	$^2P^0_{3/2}$	26364.0	4.607D+04	0.0004	0.03	26830.2	4.944D+06	0.0412	4.92
			2.679D+04	0.0002	0.02				
	$^2P^0_{1/2}$	26260.7	3.496D+06	0.0304	2.56	26723.3	1.835D+07	0.1541	18.28
			3.037D+06	0.0264	2.33				
	$^2D^0_{5/2}$	30218.5	1.110D+05	0.0007	0.08	29978.7	1.253D+06	0.0084	1.25
			2.193D+05	0.0014	0.17				
	$^2D^0_{3/2}$	29712.7	6.855D+05	0.0047	0.50	29477.8	1.370D+07	0.0945	13.64
			7.385D+05	0.0050	0.57				
$^4F_{3/2}$	$^4S^0_{3/2}$	28341.9	3.196D+07	0.2386	22.78	27993.4	3.585D+07	0.2744	17.43
			3.048D+07	0.2276	20.65				
	$^4P^0_{5/2}$	34885.3	7.035D+06	0.0347	5.01	34752.3	1.476D+07	0.0733	7.18
			7.623D+06	0.0376	5.16				
	$^4P^0_{3/2}$	34666.3	1.086D+06	0.0054	0.77	34532.5	1.074D+06	0.0054	0.52
			1.095D+06	0.0055	0.74				
	$^4P^0_{1/2}$	34486.2	9.806D+06	0.0494	6.99	34352.0	2.812D+07	0.1429	13.67
			1.058D+07	0.0534	7.17				
	$^4D^0_{5/2}$	31794.7	4.065D+01	0.0000	0.00	31494.2	6.084D+06	0.0368	2.96
			3.043D+04	0.0002	0.02				
	$^4D^0_{3/2}$	31549.0	8.801D+07	0.5303	62.73	31250.7	3.798D+07	0.2332	18.46
			9.597D+07	0.5782	65.02				
	$^4D^0_{1/2}$	31407.4	1.403D+08	0.8530	100.00	31108.8	2.057D+08	1.2747	100.00
			1.476D+08	0.8973	100.00				
	$^2S^0_{1/2}$	28481.7	6.065D+06	0.0448	4.32	28166.5	4.590D+06	0.0347	2.23
			5.692D+06	0.0421	3.86				
	$^2P^0_{3/2}$	26417.9	9.619D+06	0.0827	6.86	26778.6	3.296D+06	0.0276	1.60
			8.598D+06	0.0739	5.83				
	$^2P^0_{1/2}$	26314.6	1.973D+07	0.1709	14.06	26671.7	5.552D+05	0.0047	0.27
			1.737D+07	0.1504	11.77				
	$^2D^0_{5/2}$	30272.4	3.274D+06	0.0214	2.33	29927.1	1.378D+06	0.0092	0.67
			3.274D+06	0.0214	2.22				
	$^2D^0_{3/2}$	29766.6	1.833D+07	0.1241	1113.06	29426.3	2.957D+06	0.0205	1.44
			1.799D+07	0.1218	12.19				

Table 5
Comparison of relative branching factors: NIST [13], MCDF and MCHF

Upper	Lower	NIST	MCDF(C/B)	MCHF
$^4F_{3/2}$	$^4S^0_{3/2}$	75.28	22.78/20.65	17.43
	$^4P^0_{5/2}$	7.48	5.01/5.16	7.18
	$^4P^0_{3/2}$	0.268	0.74/0.77	0.52
	$^4P^0_{1/2}$	23.15	7.17/6.99	13.67
	$^4D^0_{5/2}$	8.837	0.00/0.02	2.96
	$^4D^0_{3/2}$	1.636	65.02/62.73	18.46
	$^4D^0_{1/2}$	100.0	100.0/100.0	100.0
	$^2S^0_{1/2}$	0.342	4.32/3.86	2.23
	$^2P^0_{3/2}$	Not obs.	6.86/5.83	1.60
	$^2P^0_{1/2}$	1.867	11.77/14.06	0.27
	$^2D^0_{5/2}$	0.118	2.33/2.22	0.67
	$^2D^0_{3/2}$	1.469	12.19/13.06	1.44

when energy levels are closely spaced or observed data is not available.

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